

## SEARCH REQUEST FORM

Scientific and Technical Information Center

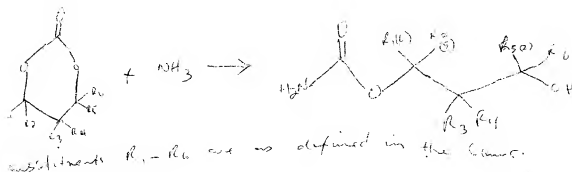
Requester's Full Name: Ben Jacey Examiner #: \_\_\_\_\_ Date: 8/26/02  
 Art Unit: 1626 Phone Number 305-8999 Serial Number: R7863550  
 Mail Box and Bldg/Room Location: CM/3E11 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

\*\*\*\*\*  
 Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc. if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Prep. of hydroxyalkyl fluoranthenes from 6,9-substituted cyclic compoundsInventors (please provide full names): John Clements et al.Earliest Priority Filing Date: 05/23/01

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.



## STAFF USE ONLY

Searcher: R. F. FisherSearcher Phone #: 708-4790

Searcher Location: \_\_\_\_\_

Date Searcher Picked Up: \_\_\_\_\_

Date Completed: 8/27/02Searcher Prep & Review Time: 20

Clerical Prep Time: \_\_\_\_\_

Online Time: 20

PTO-1590 (8-01)

## Type of Search

NA Sequence (#)

AA Sequence (#)

Structure (#)

Bibliographic

Litigation

Fulltext

Patent Family

Other

## Vendors and cost where applicable

STN

Dialog

Questel/Orbit

Dr Link

Lexis/Nexis

Sequence Systems

WWW/Internet

Other (specify)

Carbach  
 176.  $\rightarrow$  2 searches

=> FILE CASRE

FILE 'CASREACT' ENTERED AT 15:19:10 ON 29 AUG 2002  
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FILE CONTENT:1974 - 25 Aug 2002 VOL 137 ISS 8

Some records from 1974 to 1991 are derived from the ZIC/VINITI data file and provided by InfoChem.

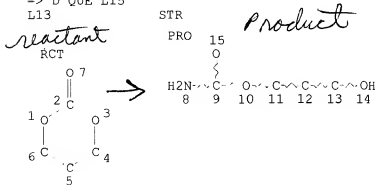
This file contains CAS Registry Numbers for easy and accurate substance identification.

Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

=> D QUE L15

L13



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

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L15          1 SEA FILE=CASREACT SSS FUL L13 (      2 REACTIONS)
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=> D L15 ALL

L15 ANSWER 1 OF 1 CASREACT COPYRIGHT 2002 ACS

AN 135:92376 CASREACT

TI Preparation of (hydroxyalkyl) carbamates via the ring-opening ammonolysis of 1,3-dioxan-2-ones

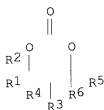
IN Clements, John H.; Klein, Howard P.; Marquis, Edward T.; Machac, James R., Jr.

PA Huntsman Petrochemical Corp., USA

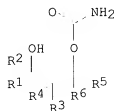
applicants

SO U.S., 6 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM C07C269-06  
 NCL 560157000  
 CC 23-20 (Aliphatic Compounds)  
 Section cross-reference(s): 45  
 FAN.CNT 1

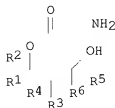
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6262297	B1	20010717	US 2000-669220	20000925
	WO 2002026700	A1	20020404	WO 2001-US16053	20010518
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BU, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
	US 2002040160	A1	20020404	US 2001-863558	20010523
PRAI	US 2000-669220		20000925		
OS	MARPAT 135:92376				
GI					



I



II



III

AB When 6-member cyclic carbonate esters [I; H, (un)branched C1-6 alkyl] are subjected to ammonolysis using either anhyd. ammonia or aq. ammonium hydroxide, (hydroxyalkyl) carbamates (II, III) are formed in high yield. Thus, 5-methyl-1,3-dioxan-2-one was reacted with anhyd. ammonia at

55.degree./140 psig, producing 2-methyl-3-hydroxypropyl carbamate in 94.5% yield.

ST dioxanone ring opening ammonolysis prepn hydroxyalkyl carbamate;  
carboxylation ring opening dioxanone prepn hydroxyalkyl carbamate

IT Carbamate esters  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(1,3-dioxan-2-ones; prepn. of (hydroxyalkyl) carbamates via the ring-opening ammonolysis of six-membered cyclic carbonates)

IT Vacuum  
(in the purifn. of (hydroxyalkyl) carbamates prepd. via the ring-opening ammonolysis of 1,3-dioxan-2-ones)

IT Carbamoylation  
(ring-opening; prepn. of (hydroxyalkyl) carbamates via the ring-opening ammonolysis of 1,3-dioxan-2-ones)

IT Ammonolysis  
(ring-opening; prepn. of (hydroxyalkyl) carbamates via the ring-opening ammonolysis of six-membered cyclic carbonates)

IT 1336-21-6, Ammonium hydroxide 7732-18-5, Water, reactions 87831-99-0, 5-Methyl-1,3-dioxan-2-one 348110-00-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of (hydroxyalkyl) carbamates via the ring-opening ammonolysis of 1,3-dioxan-2-ones)

IT 7664-41-7, Ammonia, reactions  
RL: RCT (Reactant); REM (Removal or disposal); PROC (Process); RACT (Reactant or reagent)  
(prepn. of (hydroxyalkyl) carbamates via the ring-opening ammonolysis of 1,3-dioxan-2-ones)

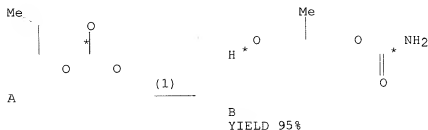
IT 17361-58-9P 31521-82-1P 348109-99-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of (hydroxyalkyl) carbamates via the ring-opening ammonolysis of 1,3-dioxan-2-ones)

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

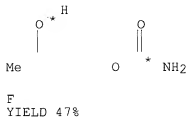
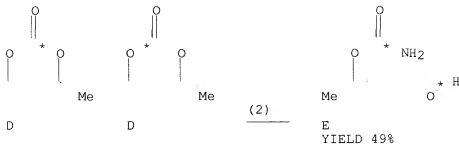
- (1) Angeles; Synthetic Communications 1994, V24(17), P2441 CAPLUS
- (2) Blank; US 4520167 1985 CAPLUS
- (3) Blank; US 4820830 1989 CAPLUS
- (4) Blank; US 5134205 1992 CAPLUS
- (5) Coury; US 4883854 1989 CAPLUS
- (6) Drysdale; US 6020499 2000 CAPLUS
- (7) Forgione; US 5089617 1992 CAPLUS
- (8) Green; International Waterborne, High-Solids, and Powder Coatings Symposium 2000
- (9) Jacobs; US 4897435 1990 CAPLUS
- (10) Parekh; US 4758632 1988 CAPLUS
- (11) Porosoff; US 5102923 1992 CAPLUS
- (12) Rehfuess; US 5605965 1997 CAPLUS

RX(1) OF 2 A ==&gt; B



RX(1) RCT A **87831-99-0**  
 RGT C 7664-41-7 NH3  
 PRO B **348109-99-9**

RX(2) OF 2 2 D ==> E + F



RX(2) RCT D **17361-58-9**  
 RGT C 7664-41-7 NH3  
 PRO E **31521-82-1**, F 348110-00-9

=> FILE REG  
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STRUCTURE FILE UPDATES: 27 AUG 2002 HIGHEST RN 445218-02-0  
 DICTIONARY FILE UPDATES: 27 AUG 2002 HIGHEST RN 445218-02-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when  
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Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES  
 for more information. See STNote 27, Searching Properties in the CAS  
 Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> FILE HCAPLUS

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FILE COVERS 1907 - 29 Aug 2002 VOL 137 ISS 9  
 FILE LAST UPDATED: 27 Aug 2002 (20020827/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> D QUE

L16 STR

15  
0

H2N- C- O- C- C- C- OH  
8 9 10 11 12 13 14

NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

L18 331 SEA FILE=REGISTRY SSS FUL L16  
 L19 499 SEA FILE=HCAPLUS ABB=ON L18  
 L20 182 SEA FILE=HCAPLUS ABB=ON L19 (L) (PREP OR IMF OR SPN)/RL  
 L21 5 SEA FILE=HCAPLUS ABB=ON L20 AND (RING?(3A)OPEN? OR RINGOPEN?)  
 L23 1 SEA FILE=REGISTRY ABB=ON 1336-21-6/RN  
 L24 10763 SEA FILE=HCAPLUS ABB=ON L23  
 L25 1 SEA FILE=REGISTRY ABB=ON 7664-41-7/RN  
 L26 99153 SEA FILE=HCAPLUS ABB=ON L25  
 L27 632427 SEA FILE=HCAPLUS ABB=ON L26 OR L24 OR NH3 OR NH4OH OR AMMON?  
 L28 27 SEA FILE=HCAPLUS ABB=ON L20 AND L27  
 L29 4 SEA FILE=HCAPLUS ABB=ON L28 AND RING?  
 L30 2 SEA FILE=HCAPLUS ABB=ON L28 AND ?DIOXAN?  
 L31 6 SEA FILE=HCAPLUS ABB=ON L28 AND CYCLIC  
 L33 13 SEA FILE=HCAPLUS ABB=ON L21 OR (L29 OR L30 OR L31)

*331 structures from this query*

*182 prep's*

=&gt; D L33 ALL 1-13 HITSTR

L33 ANSWER 1 OF 13 HCAPLUS COPYRIGHT 2002 ACS  
 AN 2002:295494 HCAPLUS  
 DN 137:109152  
 TI Studies directed toward the synthesis of the C15-C21 fragment of  
 (-)-discodermolide  
 AU Chakraborty, Tushar K.; Laxman, Pasunoori  
 CS Indian Institute of Chemical Technology, Hyderabad, 500 007, India  
 SO Journal of the Indian Chemical Society (2001), 78(10-12), 543-545  
 CODEN: JICSAH; ISSN: 0019-4522  
 PB Indian Chemical Society  
 DT Journal  
 LA English  
 CC 26-9 (Biomolecules and Their Synthetic Analogs)  
 AB A novel method developed recently for the synthesis of chiral  
 2-methyl-1,3-diols by radical-mediated diastereoselective opening of  
 trisubstituted epoxy alcs. at the more substituted carbon serves as the  
 key step in the studies directed toward the stereoselective synthesis of  
 the C15-C21 fragment of (-)-discodermolide.  
 ST discodermolide stereoselective synthesis  
 IT **Ring opening**  
 (radical, stereoselective; studies directed toward synthesis of C15-C21  
 fragment of (-)-discodermolide)  
 IT Stereoselective synthesis  
 (studies directed toward synthesis of C15-C21 fragment of  
 (-)-discodermolide)  
 IT **154335-30-5P, (-)-Discodermolide 443752-38-3P**  
 RL: PNU (Preparation, unclassified); **PREP (Preparation)**  
 (studies directed toward synthesis of C15-C21 fragment of  
 (-)-discodermolide)  
 IT 72657-23-9 160238-46-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (studies directed toward synthesis of C15-C21 fragment of  
 (-)-discodermolide)  
 IT 153775-90-7P 443752-39-4P 443752-40-7P 443752-41-8P 443752-42-9P  
 443752-43-0P 443752-44-1P 443752-45-2P 443752-46-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT  
 (Reactant or reagent)  
 (studies directed toward synthesis of C15-C21 fragment of  
 (-)-discodermolide)  
 IT 443752-47-4P 443752-48-5P  
 RL: SPN (Synthetic preparation); **PREP (Preparation)**  
 (studies directed toward synthesis of C15-C21 fragment of  
 (-)-discodermolide)  
 RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 RE  
 (1) Balachandran, R; Anticancer Drugs 1998, V9, P67 HCAPLUS  
 (2) Chakraborty, T; Chem Lett 2000, P80 HCAPLUS  
 (3) Chakraborty, T; J Chem Soc, Perkin Trans 1 1997, P1257 HCAPLUS  
 (4) Chakraborty, T; J Indian Chem Soc 1999, V76, P611 HCAPLUS  
 (5) Chakraborty, T; Tetrahedron Lett 1998, V39, P101 HCAPLUS  
 (6) Clark, D; J Org Chem 1993, V58, P5878 HCAPLUS  
 (7) Evans, D; Tetrahedron Lett 1990, V31, P7099 HCAPLUS  
 (8) Evans, D; Tetrahedron Lett 1999, V40, P4461 HCAPLUS  
 (9) Evans, P; Tetrahedron Lett 1993, V34, P8163 HCAPLUS  
 (10) Filla, S; Tetrahedron Lett 1999, V40, P5449 HCAPLUS  
 (11) Golec, J; Tetrahedron Lett 1993, V34, P8159 HCAPLUS

- IT 154335-30-5P, (-)-Discodermolide

RN 154335-30-5 HCAPLUS

CN 2H-Pyran-2-one, 6-[1

(CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



PAGE 1-B

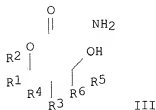
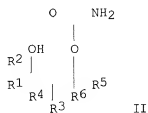
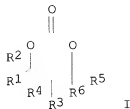
 $\text{CH}_2$



DN 135:92376  
 TI Preparation of (hydroxyalkyl) carbamates via the ring-  
 opening ammonolysis of 1,3-dioxan-2-ones  
 IN Clements, John H.; Klein, Howard P.; Marquis, Edward T.; Machac, James R.,  
 Jr.  
 PA Huntsman Petrochemical Corp., USA  
 SO U.S., 6 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM C07C269-06  
 NCL 560157000  
 CC 23-20 (Aliphatic Compounds)  
 Section cross-reference(s): 45

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6262297	B1	20010717	US 2000-669220	20000925
	WO 2002026700	A1	20020404	WO 2001-US16053	20010518
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	RW:		GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG		
	US 2002040160	A1	20020404	US 2001-863558	20010523
PRAI	US 2000-669220	A	20000925		
OS	CASREACT 135:92376; MARPAT 135:92376				
GI					



- AB When 6-member **cyclic** carbonate esters [I; H, (un)branched C1-6 alkyl] are subjected to **ammonolysis** using either anhyd. **ammonia** or aq. **ammonium hydroxide**, (hydroxyalkyl) carbamates (II, III) are formed in high yield. Thus; 5-methyl-1,3-dioxan-2-one was reacted with anhyd. **ammonia** at 55.degree./140 psig, producing 2-methyl-3-hydroxypropyl carbamate in 94.5% yield.
- ST **dioxanone ring opening ammonolysis**  
prepn hydroxyalkyl carbamate; carbonylation **ring opening dioxanone** prepn hydroxyalkyl carbamate
- IT Carbonate esters  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(1,3-dioxan-2-ones; prepn. of (hydroxyalkyl) carbamates via the **ring-opening ammonolysis** of six-membered **cyclic** carbonates)
- IT Vacuum  
(in the purifn. of (hydroxyalkyl) carbamates prepd. via the **ring-opening ammonolysis** of 1,3-dioxan-2-ones)
- IT Carbamoylation  
(**ring-opening**; prepn. of (hydroxyalkyl) carbamates via the **ring-opening ammonolysis** of 1,3-dioxan-2-ones)
- IT **Ammonolysis**  
(**ring-opening**; prepn. of (hydroxyalkyl) carbamates via the **ring-opening ammonolysis** of six-membered **cyclic** carbonates)
- IT **1336-21-6, Ammonium hydroxide** 7732-18-5, Water, reactions 87831-99-0, 5-Methyl-1,3-dioxan-2-one 348110-00-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of (hydroxyalkyl) carbamates via the **ring-opening ammonolysis** of 1,3-dioxan-2-ones)
- IT **7664-41-7, Ammonia**, reactions  
RL: RCT (Reactant); REM (Removal or disposal); PROC (Process); RACT (Reactant or reagent)  
(prepn. of (hydroxyalkyl) carbamates via the **ring-opening ammonolysis** of 1,3-dioxan-2-ones)
- IT 17361-58-9P 31521-82-1P 348109-99-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of (hydroxyalkyl) carbamates via the **ring-opening ammonolysis** of 1,3-dioxan-2-ones)
- RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
- RE
- (1) Angeles; Synthetic Communications 1994, V24(17), P2441 HCAPLUS
  - (2) Blank; US 4520167 1985 HCAPLUS
  - (3) Blank; US 4820830 1989 HCAPLUS
  - (4) Blank; US 5134205 1992 HCAPLUS
  - (5) Coury; US 4883854 1989 HCAPLUS
  - (6) Drysdale; US 6020499 2000 HCAPLUS
  - (7) Forgiione; US 5089617 1992 HCAPLUS
  - (8) Green; International Waterborne, High-Solids, and Powder Coatings Symposium 2000
  - (9) Jacobs; US 4897435 1990 HCAPLUS
  - (10) Parekh; US 4758632 1988 HCAPLUS
  - (11) Porosoff; US 5102923 1992 HCAPLUS
  - (12) Rehfuss; US 5605965 1997 HCAPLUS
- IT **1336-21-6, Ammonium hydroxide**  
RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of (hydroxyalkyl) carbamates via the ring-opening amonolysis of 1,3-dioxan-2-ones)

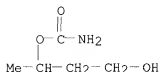
RN 1336-21-6 HCAPLUS  
CN Ammonium hydroxide ((NH4)(OH)) (9CI) (CA INDEX NAME)

H4N-OH

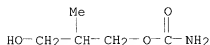
IT 7664-41-7, Ammonia, reactions  
RL: RCT (Reactant); REM (Removal or disposal); PROC (Process); RACT (Reactant or reagent)  
(prepn. of (hydroxyalkyl) carbamates via the ring-opening amonolysis of 1,3-dioxan-2-ones)  
RN 7664-41-7 HCAPLUS  
CN Ammonia (8CI, 9CI) (CA INDEX NAME)

NH3

IT 31521-82-1P 348109-99-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of (hydroxyalkyl) carbamates via the ring-opening amonolysis of 1,3-dioxan-2-ones)  
RN 31521-82-1 HCAPLUS  
CN 1,3-Butanediol, 3-carbamate (8CI, 9CI) (CA INDEX NAME)



RN 348109-99-9 HCAPLUS  
CN 1,3-Propanediol, 2-methyl-, monocarbamate (9CI) (CA INDEX NAME)



L33 ANSWER 3 OF 13 HCAPLUS COPYRIGHT 2002 ACS

AN 1999:566027 HCAPLUS

DN 131:184942

TI Preparation of 3-(5-isoxazolyl)- or 3-phenylpropylamine derivatives as central muscle relaxants

IN Matsui, Takeaki; Tanaka, Yuichiro; Inoue, Masaki; Etoh, Shugo; Noda, Masatoshi; Yabuki, Tetsuaki; Toga, Tetsuo; Amagishi, Hiroaki; Hayakawa, Maki; Tanaka, Chikage; Matsumura, Yumi

PA Maruho Kabushikikaisha, Japan

SO PCT Int. Appl., 66 pp.

CODEN: PIXXD2

DT Patent

LA Japanese

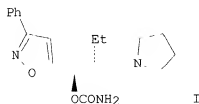
IC ICM C07D211-14

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ICS C07D261-08; C07D277-28; C07D295-092; C07D307-52; C07D307-81;  
C07D333-20; C07D333-58; A61K031-40; A61K031-42; A61K031-425;  
A61K031-445; A61K031-535; A61K031-55  
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9943656	Al	19990902	WO 1999-JP759	19990219
	W: CN, JP, KR, US				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRAI	JP 1998-43998		19980225		
OS	MARPAT 131:184942				
GI					



- AB Propylamine derivs. represented by formula ACH(O2CNHR5)CR1R2CH2NR3R4 and salts thereof (wherein A is substituted aryl or optionally substituted heteroaryl; R1 and R2 are the same or different lower alkyls, or one of R1 and R2 is hydrogen and the other is lower alkyl, lower alkoxy, aryl, aralkyl, or lower alkoxy- or lower alkylthio-substituted lower alkyl; one of R3 and R4 is hydrogen or lower alkyl and the other is lower cycloalkyl, or R3 or R4 are the same or different lower alkyls or are bonded to each other to form a ring which contains one or more nitrogen or oxygen atoms and is optionally substituted by lower alkyl, lower alkanoyl, or aralkyl; and R5 is hydrogen, lower alkyl, or aryl) are prepd. These compds. are useful as central muscle relaxants or for the treatment of urination disorders. Thus, (1R,2R)-5-[1-hydroxy-2-(1-pyrrolidinylmethyl)butyl]-3-phenylisoxazole was condensed with Ph chlorocarbonate in pyridine/CH2Cl2 at room temp. for 2 h and the amidated with NH3 in 2-propanol at room temp. for 4 h to give, after salt formation with oxalic acid, (1R,2R)-5-[1-(carbamoyloxy)-2-(1-pyrrolidinylmethyl)butyl]-3-phenylisoxazole [1.(CO2H)2]. I.(CO2H)2 at 4.0 mg/kg p.o. relaxed 84.7% decerebrate rigidity in rats.
- ST isoxazolypropylamine prepn central muscle relaxant; urination disorder treatment carbamoyloxy-pyrrolidinylmethylbutylphenylisoxazole; phenylisoxazole carbamoyloxy pyrrolidinylmethyl butyl prepn; phenylpropylamine prepn central muscle relaxant
- IT Muscle relaxants  
(central; prepn. of (isoxazoly)propylamine derivs. as central muscle relaxants and for treatment of urination disorders)
- IT Micturition  
(disorder; prepn. of (isoxazoly)propylamine derivs. as central muscle relaxants and for treatment of urination disorders)
- IT 240123-98-2P 240124-01-0P 240124-04-3P 240124-08-7P 240124-12-3P  
240124-14-5P 240124-16-7P 240124-17-8P 240124-20-3P 240124-22-5P  
240124-23-6P 240124-25-8P 240124-26-9P 240124-29-2P 240124-31-6P  
240124-32-7P 240124-33-8P 240124-34-9P 240124-55-4P 240124-56-5P  
240124-57-6P 240124-58-7P 240124-61-2P 240404-84-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of (isoxazolyl)propylamine derivs. as central muscle relaxants and for treatment of urination disorders)

- IT 75-04-7, Ethylamine, reactions 98-59-9, p-Toluenesulfonyl chloride  
103-71-9, Phenyl isocyanate, reactions 123-75-1, Pyrrolidine, reactions  
141-75-3, n-Butyryl chloride 17016-83-0, (S)-4-Isopropylloxazolidin-2-one  
64840-90-0 72418-40-7 95530-58-8, (R)-4-Isopropylloxazolidin-2-one  
145588-94-9 166740-28-9 166740-30-3 166740-32-5 179077-80-6  
240124-65-6 240124-67-8 240124-68-9 240124-69-0 240124-70-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of (isoxazolyl)propylamine derivs. as central muscle relaxants and for treatment of urination disorders)

- IT 157796-13-9P 240124-27-0P 240124-28-1P 240124-30-5P 240124-35-0P  
240124-36-1P 240124-37-2P 240124-38-3P 240124-39-4P  
240124-40-7P 240124-41-8P 240124-42-9P 240124-43-0P  
240124-44-1P 240124-45-2P 240124-46-3P 240124-47-4P  
240124-48-5P 240124-49-6P 240124-50-9P 240124-51-0P  
240124-52-1P 240124-53-2P 240124-54-3P 240124-59-8P  
240124-60-1P 240124-62-3P 240124-63-4P 240124-64-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(prepn. of (isoxazolyl)propylamine derivs. as central muscle relaxants and for treatment of urination disorders)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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- (3) Bayer Ag; EP 40740 A HCAPLUS
- (4) Bayer Ag; US 4495184 A HCAPLUS
- (5) Bayer Ag; JP 5716841 A 1982

IT 240124-38-3P 240124-43-0P 240124-48-5P

240124-53-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

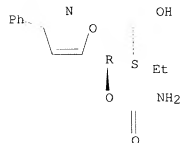
(Preparation); RACT (Reactant or reagent)

(prepn. of (isoxazolyl)propylamine derivs. as central muscle relaxants and for treatment of urination disorders)

RN 240124-38-3 HCAPLUS

CN 1,3-Propanediol, 2-ethyl-1-(3-phenyl-5-isoxazolyl)-, 1-carbamate, (1R,2S)-(9CI) (CA INDEX NAME)

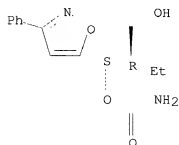
Absolute stereochemistry. Rotation (+).



RN 240124-43-0 HCAPLUS

CN 1,3-Propanediol, 2-ethyl-1-(3-phenyl-5-isoxazolyl)-, 1-carbamate, (1S,2R)-(9CI) (CA INDEX NAME)

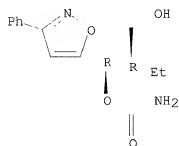
Absolute stereochemistry. Rotation (-).



RN 240124-48-5 HCAPLUS

CN 1,3-Propanediol, 2-ethyl-1-(3-phenyl-5-isoxazolyl)-, 1-carbamate, (1R,2R)-(9CI) (CA INDEX NAME)

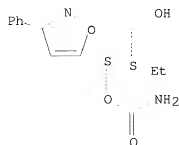
Absolute stereochemistry. Rotation (+).



RN 240124-53-2 HCAPLUS

CN 1,3-Propanediol, 2-ethyl-1-(3-phenyl-5-isoxazolyl)-, 1-carbamate, (1S,2S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L33 ANSWER 4 OF 13 HCAPLUS COPYRIGHT 2002 ACS

AN 1999:286766 HCAPLUS

DN 131:129813

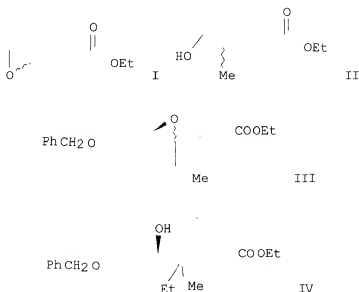
TI Natural product synthesis based on the stereospecific acyclic stereocontrol

AU Miyazawa, Masahiro; Maruyama, Kimiyuki; Sasaki, Shinobu; Ohnuma, Satoshi; Ishibashi, Naoki; Sasaki, Minoru; Miyashita, Masaaki

CS Graduate School of Science, Hokkaido University, Japan

SO Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1998), 40th, 211-216

CODEN: TYKYDS  
 PB Nippon Kagakkai  
 DT Journal  
 LA Japanese  
 CC 26-9 (Biomolecules and Their Synthetic Analogs)  
 GI



AB The authors recently developed a novel acyclic stereocontrol based on the stereospecific methylation of .gamma.,.delta.-epoxy acrylates with trimethylaluminum in the presence of water by which both anti and syn compds. can be highly stereoselectively synthesized from trans- and cis-.gamma.,.delta.-epoxy acrylates, resp. The authors report here stereospecific internal alkylation of terminal epoxides and stereospecific construction of asym. quaternary carbons via .gamma.,.delta.-epoxy acrylates. The authors also report synthetic studies toward total synthesis of a marine natural product discodermolide and epothilone based on the above methodologies. Regio- and stereoselective internal alkylation of terminal epoxides has little been known. The authors designed such a reaction using .gamma.,.delta.-epoxy acrylates with trimethylaluminum. The reaction of terminal .gamma.,.delta.-epoxy acrylates (S)- and (R)-I, easily prep'd. from D-mannitol, with excess trimethylaluminum in the presence of water proceeded regiospecifically at the .gamma.-position to give (R)- and (S)-II, as the sole product, resp., with maintenance of optical integrity. Regarding stereospecific construction of asym. quaternary carbons via .gamma.-Alkyl-.gamma.,.delta.-epoxy acrylates, the authors found that the reaction of .gamma.-alkyl-.gamma.,.delta.-epoxy acrylates with trialkylaluminum and water occurs regio- and stereo-specifically at the .gamma.-position as well yielding an asym. quaternary carbon. Thus, treatment of (4R)- and (4S)-III with excess trimethylaluminum in the presence of water gave (4R)- and (4S)-IV as a single product, resp., in which a Me group was stereospecifically introduced at the .gamma.-position with net inversion of configuration. Regarding synthetic studies on discodermolide and epothilone, the authors set out synthesis of discodermolide having potent immunosuppressive activity based on the above stereospecific acyclic stereocontrol. Discodermolide was divided into three segments in which

the segment B having three contiguous chiral centers and the segment C possessing five chiral centers have been highly stereoselectively synthesized. Stereoselective synthesis of the C1-C9 segment of epothilone having potent anticancer activity was also carried out in which five asymmetric centers was highly stereoselectively constructed by repeating the above methylation reaction.

ST stereospecific acyclic stereocontrol natural product synthesis

IT Natural products

RL: SPN (Synthetic preparation); PREP (Preparation)  
(natural product synthesis based on stereospecific acyclic stereocontrol)

IT Alkylation

(stereoselective; natural product synthesis based on stereospecific acyclic stereocontrol)

IT 191275-35-1 191275-36-2 234769-47-2 234769-48-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
(natural product synthesis based on stereospecific acyclic stereocontrol)

IT 127943-53-7P, Discodermolide 152044-53-6DP, Epothilone a, analogs 191275-37-3P 191275-38-4P 234769-49-4P 234769-50-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(natural product synthesis based on stereospecific acyclic stereocontrol)

IT 75-24-1, Trimethyl aluminum

RL: RCT (Reactant); RACT (Reactant or reagent)  
(stereospecific alkylation and epoxide ring opening by)

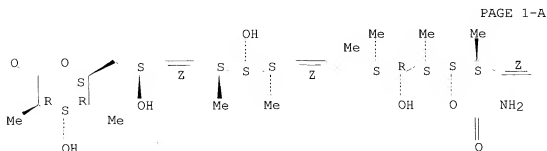
IT 127943-53-7P, Discodermolide

RL: SPN (Synthetic preparation); PREP (Preparation)  
(natural product synthesis based on stereospecific acyclic stereocontrol)

RN 127943-53-7 HCAPLUS

CN 2H-Pyran-2-one, 6-[(2S,3Z,5S,6S,7S,8Z,11S,12R,13S,14S,15S,16Z)-14-[(aminocarbonyl)oxy]-2,6,12-trihydroxy-5,7,9,11,13,15-hexamethyl-3,8,16,18-nonadecatetraenyl]tetrahydro-4-hydroxy-3,5-dimethyl-, (3R,4S,5R,6S)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



CH<sub>2</sub>



L33 ANSWER 5 OF 13 HCAPLUS COPYRIGHT 2002 ACS  
 AN 1999:202358 HCAPLUS  
 DN 130:267674  
 TI Total Synthesis of (+)-Polyoxin J  
 AU Ghosh, Arun K.; Wang, Yong  
 CS Department of Chemistry, University of Illinois at Chicago, Chicago, IL, 60607, USA  
 SO Journal of Organic Chemistry (1999), 64(8), 2789-2795  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PB American Chemical Society  
 DT Journal  
 LA English  
 CC 33-7 (Carbohydrates)  
 OS CASREACT 130:267674  
 AB Stereoselective total synthesis of (+)-polyoxin J is described. The synthesis was achieved in a convergent manner by coupling protected thymine polyoxin C and 5-O-carbamoyl polyoxamic acid and subsequent removal of the protecting groups. The key steps of the synthesis of protected thymine polyoxin C involved the stereoselective electrophilic epoxidn. of an E-allyl alc. derived from isopropylidene D-ribose deriv., followed by regioselective epoxide opening of the syn-epoxide and conversion of resulting azido diol to protected thymine polyoxin C. Protected polyoxamic acid was synthesized stereoselectively by utilizing Sharpless epoxidn. of a tartrate-derived allylic alc. followed by a regioselective epoxide **ring opening** with diisopropoxytitanium diazide.  
 ST thymine polyoxin C stereoselective epoxidn regioselective epoxide opening; polyoxin J stereoselective total synthesis  
 IT **Ring opening**  
 (regioselective; total synthesis of (+)-polyoxin J)  
 IT Epoxidation  
 (stereoselective; total synthesis of (+)-polyoxin J)  
 IT 65-71-4, Thymine 108818-00-4 131121-18-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (total synthesis of (+)-polyoxin J)  
 IT 58934-84-2P 90661-54-4P 105309-43-1P 127257-35-6P 127646-34-8P  
 130193-61-2P 143833-90-3P 155023-01-1P 213973-65-0P 222400-52-4P  
 222400-53-5P 222400-54-6P 222400-56-8P 222400-57-9P 222403-61-4P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (total synthesis of (+)-polyoxin J)  
 IT **22976-89-2P** 143833-91-4P 222400-55-7P  
 RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (total synthesis of (+)-polyoxin J)  
 RE.CNT 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 RE  
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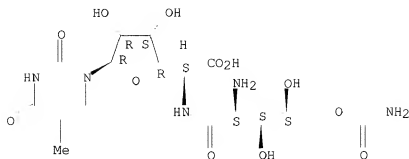
IT 22976-89-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(total synthesis of (+)-polyoxin J)

RN 22976-89-2 HCAPLUS

CN .beta.-D-Allofuranuronic acid, 5-[[[2-amino-5-O-(aminocarbonyl)-2-deoxy-L-xylonoyl]amino]-1,5-dideoxy-1-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L33 ANSWER 6 OF 13 HCAPLUS COPYRIGHT 2002 ACS

AN 1997:421294 HCAPLUS

DN 127:34005

TI Novel sulfamate compounds containing an N-substituted carbamoyl group, useful as CNS drugs, and method for preparing them

IN Choi, Yong Moon; Han, Dong Il; Kim, Hyung Cheol

PA Yukong Limited, S. Korea

SO PCT Int. Appl., 146 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM C07C307-02

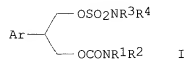
ICS A61K031-27

CC 25-21 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

Section cross-reference(s): 1

FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9716418	A1	19970509	WO 1996-KR190	19961101
	W: CA, CN, JP				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	CA 2209229	AA	19970509	CA 1996-2209229	19961101
	EP 801642	A1	19971022	EP 1996-935567	19961101
	EP 801642	B1	20001220		
	R: BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE, PT, IE				
	CN 1173864	A	19980218	CN 1996-191830	19961101
	CN 1077570	B	20020109		
	JP 10512591	T2	19981202	JP 1996-517235	19961101
	ES 2154840	T3	20010416	ES 1996-935567	19961101
PRAI	KR 1995-39456	A	19951102		
	KR 1996-49052	A	19961028		
	WO 1996-KR190	W	19961101		
OS	MARPAT 127:34005				
GI					



AB Novel sulfamate compds. contg. an N-substituted carbamoyl group are disclosed, specifically I [Ar = (un)substituted Ph; R<sup>1</sup>, R<sup>2</sup>, R<sup>3</sup>, R<sup>4</sup> = H,

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alkyl, cycloalkyl, aryl; or NR1R2 and/or NR3R4 may form 3- to 7-membered aliph. **cyclic** structure(s) with another N or O atom), including both their racemates and (R)- and (S)-optical isomers. I are useful for the prophylaxis and treatment of disorders of the central nervous system, esp. nervous myalgia, epilepsy, and minimal brain dysfunction (no data). For instance, reaction of  $\text{AcOCH}_2\text{CHPhCH}_2\text{OH}$  with carbonyldiimidazole in  $\text{CH}_2\text{Cl}_2$  and then with aq.  $\text{NH}_3$  gave 95%  $\text{AcOCH}_2\text{CHPhCH}_2\text{OCONH}_2$ . This compd. was deacetylated with KCN in MeOH (88%), and the resultant alc. was sulfamoylated with  $\text{ClSO}_2\text{NH}_2$  in pyridine (85%), to give title compd.  $\text{H}_2\text{NSO}_2\text{OCH}_2\text{CHPhCH}_2\text{OCONH}_2$ . A variety of substituted I, including (R)- and (S)-isomers, were prepd. by this and other methods.

- ST phenylpropanediol carbamate sulfamate prepn CNS drug; antiepileptic  
propanediol carbamate sulfamate prepn
- IT Muscle, disease  
(myalgia, treatment; prepn. of phenylpropanediol carbamate sulfamate compds. as CNS agents)
- IT Cytoprotective agents  
(neuroprotectants; prepn. of phenylpropanediol carbamate sulfamate compds. as CNS agents)
- IT Anticonvulsants  
Nervous system agents  
(prepn. of phenylpropanediol carbamate sulfamate compds. as CNS agents)
- IT Brain, disease  
(stroke, treatment; prepn. of phenylpropanediol carbamate sulfamate compds. as CNS agents)
- IT Brain  
(treatment of minimal dysfunction; prepn. of phenylpropanediol carbamate sulfamate compds. as CNS agents)

- IT **25451-53-OP 171433-01-5P 171433-04-8P**
- |              |              |              |              |              |
|--------------|--------------|--------------|--------------|--------------|
| 178759-04-1P | 178759-44-9P | 190589-95-8P | 190589-96-9P | 190589-97-0P |
| 190589-98-1P | 190589-99-2P | 190590-00-2P | 190590-01-3P | 190590-03-5P |
| 190590-04-6P | 190590-05-7P | 190590-06-8P | 190590-07-9P | 190590-08-0P |
| 190590-16-0P | 190590-17-1P | 190590-19-3P | 190590-20-6P | 190590-21-7P |
| 190590-22-8P | 190590-23-9P | 190590-24-0P | 190590-25-1P | 190590-26-2P |
| 190590-27-3P | 190590-28-4P | 190590-29-5P | 190590-30-8P | 190590-38-6P |
| 190590-39-7P | 190590-47-7P | 190590-48-8P | 190590-49-9P | 190590-50-2P |
| 190590-51-3P | 190590-52-4P | 190590-53-5P | 190590-54-6P | 190590-55-7P |
| 190590-56-8P | 190590-57-9P | 190590-58-0P |              |              |

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of phenylpropanediol carbamate sulfamate compds. as CNS agents)

- IT 190590-09-1P 190590-10-4P 190590-11-5P 190590-12-6P 190590-13-7P  
190590-14-8P 190590-15-9P 190590-18-2P 190590-31-9P 190590-32-0P  
190590-33-1P 190590-34-2P 190590-35-3P 190590-36-4P 190590-37-5P  
190590-41-1P 190590-42-2P 190590-43-3P 190590-44-4P 190590-45-5P  
190590-46-6P 190590-59-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of phenylpropanediol carbamate sulfamate compds. as CNS agents)

- IT 74-89-5, Methylamine, reactions 75-31-0, Isopropylamine, reactions 103-71-9, Phenyl isocyanate, reactions 110-91-8, Morpholine, reactions 124-40-3, Dimethylamine, reactions 530-62-1 765-30-0, Cyclopropylamine 7778-42-9, Sulfamoyl chloride 110230-69-8 110270-51-4 126986-28-5  
190590-60-4 190590-61-5 190897-00-8

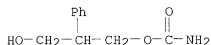
RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; prepn. of phenylpropanediol carbamate sulfamate compds. as CNS agents)

- IT **25451-53-OP 171433-01-5P 171433-04-8P**

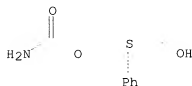
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)  
(intermediate; prepn. of phenylpropanediol carbamate sulfamate compds.  
as CNS agents)

RN 25451-53-0 HCAPLUS  
CN 1,3-Propanediol, 2-phenyl-, monocarbamate (8CI, 9CI) (CA INDEX NAME)



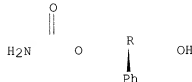
RN 171433-01-5 HCAPLUS  
CN 1,3-Propanediol, 2-phenyl-, monocarbamate, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

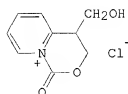


RN 171433-04-8 HCAPLUS  
CN 1,3-Propanediol, 2-phenyl-, monocarbamate, (2R)- (9CI) (CA INDEX NAME)

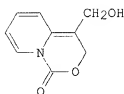
Absolute stereochemistry.



L33 ANSWER 7 OF 13 HCAPLUS COPYRIGHT 2002 ACS  
AN 1992:570572 HCAPLUS  
DN 117:170572  
TI Unique carbamation of 2-(2-pyridyl)-1,3-propanediol by phosgenation  
followed by **ammonolysis**  
AU Choi, Yong Moon; Rosso, Victor; Kucharczyk, Norbert; Sofia, R. Duane  
CS Wallace Lab., Cranbury, NJ, 08512, USA  
SO J. Org. Chem. (1992), 57(21), 5764-6  
CODEN: JOCEAH; ISSN: 0022-3263  
DT Journal  
LA English  
CC 22-4 (Physical Organic Chemistry)  
Section cross-reference(s): 27  
OS CASREACT 117:170572  
GI



I



II

- AB The unique phosgenation between 2-(2-pyridyl)-1,3-propanediol and ClCOCl in pyridine or THF contg. Et3N makes available intramol. **cyclic**, 1H-pyrido[1,2-c][1,3]-3,4-dihydro-4-(hydroxymethyl)-1-oxooxazinium chloride salt (I) which is characterized. **NH3** reacts with I to give RCH(CH2OH)CH2O2CNH2 (R = 2-pyridyl). The combined reactions (phosgenation and **ammonolysis**), thus, are systematically studied and compared at 0.degree., -30.degree., and -70.degree.. The unexpected products, the deprotonated second **cyclic** intermediate, 1H,3H-pyrido[1,2-c][1,3]oxazin-4-hydroxymethyl-1-one (II) and 2-(2-pyridyl)-3-hydroxypropene, are derived from the salt-like intermediate by .alpha.-proton abstraction. At an appropriate lower temp. the carbamation successfully competes with the .alpha.-proton abstraction.
- ST carbamation pyridylpropanediol mechanism; phosgenation **ammonolysis** pyridylpropanediol; pyridooxazinium chloride **ammonolysis**
- IT **Ring** cleavage  
(of pyridodihydro(hydroxymethyl)oxooxazinium chloride by **ammonia**, deprotonation vs.)
- IT Cyclocondensation reaction  
(of pyridylpropanediol with phosgene)
- IT **Ammonolysis**  
(phosgenation and, of pyridylpropanediol, mechanism of)
- IT Protonation and Proton transfer reaction  
(deprotonation, of pyridodihydro(hydroxymethyl)oxooxazinium chloride by **ammonia** or amines, **ring** cleavage and)
- IT Acylation  
(phosgenation, **ammonolysis** and, for carbamation of pyridylpropanediol, mechanism of)
- IT **7664-41-7**  
RL: RCT (Reactant)  
(**ammonolysis**, phosgenation and, of pyridylpropanediol, mechanism of)
- IT 49745-42-8, 2-(2-Pyridyl)-1,3-propanediol  
RL: RCT (Reactant)  
(carbamation of, with phosgene in presence of triethylamine, mechanism of)
- IT 75-44-5, Phosgene  
RL: RCT (Reactant)  
(carbamation with, of pyridylpropanediol)
- IT 137518-88-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and **ring** cleavage and deprotonation of, mechanism of)
- IT 554-68-7P, Triethylamine hydrochloride 58379-60-5P 137094-10-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)
- IT **86199-37-3P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, mechanism of)
- IT 12408-02-5  
RL: RCT (Reactant)

(protonation and Proton transfer reaction, deprotonation, of pyridodihydro(hydroxymethyl)oxoxazinium chloride by ammonia or amines, ring cleavage and)

IT 7664-41-7

RL: RCT (Reactant)

(**ammonolysis**, phosgenation and, of pyridylpropanediol, mechanism of)

RN 7664-41-7 HCAPLUS

CN Ammonia (8CI, 9CI) (CA INDEX NAME)

NH<sub>3</sub>

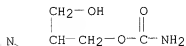
IT 86199-37-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, mechanism of)

RN 86199-37-3 HCAPLUS

CN 1,3-Propanediol, 2-(2-pyridinyl)-, monocarbamate (ester) (9CI) (CA INDEX NAME)



L33 ANSWER 8 OF 13 HCAPLUS COPYRIGHT 2002 ACS

AN 1989:439851 HCAPLUS

DN 111:39851

TI Preparation and testing of bactericidal .alpha.-hydroxy-.beta.-lysine derivatives

IN Masuya, Hiromoto; Harada, Setsuo; Natsugari, Hideaki

PA Takeda Chemical Industries, Ltd., Japan

SO Eur. Pat. Appl., 120 pp.

CODEN: EPXXDW

DT Patent

LA English

IC ICM C07C123-00

ICS C07C125-065; C07C103-66; C07C109-08; C07D295-12; C07D295-18;  
C07F007-18; A61K031-155; A61K031-27; A61K031-16; A61K031-195

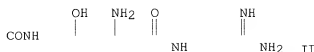
CC 34-2 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 1, 16

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 271829	A2	19880622	EP 1987-118314	19871210
	EP 271829	A3	19890726		
	EP 271829	B1	19930825		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	JP 63277652	A2	19881115	JP 1987-306382	19871202
	AT 93513	E	19930915	AT 1987-118314	19871210
PRAI	JP 1986-294432		19861210		
	JP 1987-306382		19871202		
	EP 1987-118314		19871210		
OS	MARPAT 111:39851				

GI



- AB R1CHR2CH(OR3)CH2CHR4CH2COR5 [I; R1, R4 = (substituted) amino; R2 = H, (substituted) alkyl; R3 = H, protecting group; R5 = OH, amino, etc.] useful as antibacterials, were prepd. H2NCH2CH(OH)CH2CH(NHBOC)CH2CONHCH2C(=O)NH2.2HCl (BOC = Me3CO2C) in DMF was acylated by crotonic acid in the presence of Et3N/DCC/hydroxybenzotriazole and the product was deprotected with CF3CO2H to give .delta.-hydroxy-.beta.-lysine deriv. II. Several II had MIC's of 100 .mu.g/mL against *Streptococcus aureus* 308A-I and ED50's in mice of 4.42-25 mg/kg s.c.
- ST hydroxybetalysine deriv prepn antibacterial; bactericide  
alkenylcarbonylhydroxybetalysine; lysine hydroxybeta prepn antibacterial;  
amino acid deriv hydroxylysine prepn bactericide
- IT Yeast  
(chiral redn. by, of ketoaminobutyrate deriv.)
- IT *Pseudomonas acidovorans*  
(deacylation by, of hydroxylysine deriv., in prepn. of bactericide)
- IT *Pseudomonas fluorescens*  
(hydroxylysine deriv. manuf. with, in prepn. of bactericide)
- IT Bactericides, Disinfectants, and Antiseptics  
(hydroxylysine derivs.)
- IT Asymmetric synthesis and induction  
(of hydroxylysine bactericides)
- IT Amino acids, preparation  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(derivs., hydroxylysine, prepn. of, as bactericides)
- IT 501-53-1, Carbobenzoxy chloride 17341-93-4, 2,2,2-Trichloroethoxycarbonyl chloride  
RL: RCT (Reactant)  
(acylation by, of amino lactone deriv., in prepn. of bactericide)
- IT 98-88-4, Benzoyl chloride 501-53-1, Benzyloxycarbonyl chloride 2614-88-2 3724-65-0, 2-Butenoic acid  
RL: RCT (Reactant)  
(acylation by, of hydroxylysine deriv., in prepn. of bactericide)
- IT 110-44-1, Sorbic acid 91028-39-6  
RL: RCT (Reactant)  
(acylation by, of .beta.-lysine deriv., in prepn. of bactericide)
- IT 60099-09-4, Benzyl formimidate hydrochloride 113904-16-8  
RL: RCT (Reactant)  
(amidation by, of hydroxylysine deriv., in prepn. of bactericide)
- IT 82353-56-8  
RL: RCT (Reactant)  
(chiral cyclocondensation of, with silyloxydiene deriv.)
- IT 38330-80-2, Potassium monomethyl malonate  
RL: RCT (Reactant)  
(condensation of, with alanine deriv.)
- IT 7803-57-8, Hydrazine hydrate 51127-12-9 60099-09-4, Benzyl formimidate hydrochloride 82102-87-2 107819-90-9 119962-71-9  
RL: RCT (Reactant)  
(condensation of, with hydroxylysine deriv., in prepn. of bactericide)
- IT 15761-38-3, BOC-Ala-OH  
RL: RCT (Reactant)



- (condensation of, with malonate)  
 IT 3850-40-6 4530-20-5 7764-95-6 15761-38-3 119962-72-0  
 RL: RCT (Reactant)  
 (condensation of, with .beta.-amino lysine deriv., in prepn. of bactericide)  
 IT 3262-72-4  
 RL: RCT (Reactant)  
 (condensation of, with .beta.-lysine deriv., in prepn. of bactericide)  
 IT 105-45-3, Methyl acetoacetate  
 RL: PROC (Process)  
 (conversion of, to silyl enol ether)  
 IT 111408-79-8  
 RL: RCT (Reactant)  
 (hydrogenation of, in prepn. of bactericide)  
 IT 111337-84-9 111337-85-0 111337-86-1 111465-40-8  
 RL: RCT (Reactant)  
 (manuf. with *Pseudomonas fluorescens*, in synthesis of bactericides)  
 IT 74-88-4, Methyl iodide, reactions  
 RL: RCT (Reactant)  
 (methylation of, of hydroxylysine deriv., in prepn. of bactericide)  
 IT 119962-69-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and condensation of, with aminopimelic acid deriv.)  
 IT 67609-52-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and cyclocondensation of, with alaninal deriv., in prepn. of bactericide)  
 IT 119960-28-0P 119960-29-1P 119960-30-4P 119960-31-5P 119960-32-6P  
 119960-33-7P 119960-34-8P 119960-35-9P 119960-36-0P 119960-37-1P  
 119960-38-2P 119960-39-3P 119960-40-6P 119960-41-7P 119960-42-8P  
 119960-43-9P 119960-44-0P 119960-45-1P 119960-46-2P 119960-47-3P  
 119960-48-4P 119960-49-5P 119960-50-8P **119960-51-9P**  
 119960-52-0P 119960-53-1P 119960-54-2P 119960-55-3P 119960-56-4P  
 119960-57-5P 119960-58-6P 119960-59-7P 119960-60-0P 119960-61-1P  
 119962-70-8P 119962-96-8P 119976-64-6P 119976-65-7P 119976-91-9P  
 119996-78-0P 120021-40-1P 120021-41-2P 120021-42-3P 120021-55-8P  
 120053-43-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (Preparation)  
 (prepn. and deprotection of, in prepn. of bactericide)  
 IT 119962-97-9P 119962-98-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and deprotection of, in prepn. of hydroxylysine bactericide)  
 IT 111305-50-1P 119960-62-2P 119960-63-3P 119960-64-4P 119960-65-5P  
 119960-66-6P 119960-67-7P 119960-68-8P 119960-69-9P 119960-70-2P  
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and reaction of, in prepn. of bactericide)

IT 119962-89-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and reaction of, in prepn. of hydroxyllysine bactericide)

IT	111337-87-2P	111337-88-3P	119960-27-9P	119961-35-2P	119961-36-3P
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	119961-57-8P	119961-58-9P	119961-59-0P	119961-60-3P	
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	119961-67-0P	119961-68-1P	119961-69-2P	119961-70-5P	119961-71-6P
	119961-72-7P	119961-73-8P	119961-74-9P	119961-75-0P	119961-76-1P
	119961-77-2P	119961-78-3P	119961-79-4P	119961-80-7P	119961-81-8P
	119961-82-9P	119961-83-0P	119961-84-1P	119961-85-2P	119961-86-3P
	119961-87-4P	119961-88-5P	119961-89-6P	119961-90-9P	119961-91-0P
	119961-92-1P	119961-93-2P	119961-94-3P	119961-95-4P	119961-96-5P
	119961-97-6P	119961-98-7P	119961-99-8P	119962-01-5P	119962-02-6P
	119962-03-7P	119962-04-8P	119962-05-9P	119962-06-0P	119962-07-1P
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	120021-53-6P	120021-54-7P	120053-44-3P	120053-45-4P	120053-46-5P

RL: BAC (Biological activity or effector, except adverse); SPN  
(Synthetic preparation); BIOL (Biological study); PREP  
(Preparation)

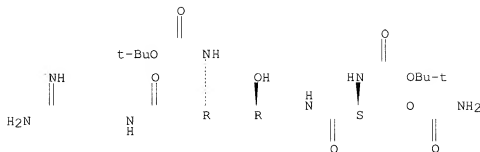
(prepn. of, as bactericide)

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	111305-65-8P	111305-68-1P	111305-71-6P	111305-72-7P	111305-74-9P
	111305-75-0P	111305-77-2P	111305-79-4P	111305-80-7P	111407-96-6P
	119959-98-7P	119959-99-8P	119960-00-8P	119960-01-9P	119960-02-0P
	119960-03-1P	119960-04-2P	119960-05-3P	119960-06-4P	119960-07-5P
	119960-08-6P	119960-09-7P	119960-10-0P	119960-11-1P	119960-12-2P
	119960-13-3P	119960-14-4P	119960-15-5P	119960-16-6P	119960-17-7P
	119960-18-8P	119960-19-9P	119960-20-2P	119960-21-3P	119960-22-4P
	119960-23-5P	119960-24-6P	119960-25-7P	119960-26-8P	119960-27-9P
	119962-73-1P	119962-74-2P	119962-75-3P	119962-76-4P	119962-77-5P
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	119962-83-3P	119962-84-4P	119962-85-5P	119962-86-6P	119962-87-7P
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	120021-29-6P	120021-30-9P	120021-31-0P	120021-32-1P	120021-33-2P
	120021-34-3P	120021-35-4P	120021-36-5P	120021-37-6P	120021-38-7P
	120021-39-8P	120052-38-2P			

RL: SPN (Synthetic preparation); PREP (Preparation)

- (prepn. of, as bactericide intermediate)
- IT 119963-01-8P 119963-02-9P 119963-03-0P 119963-04-1P 119963-05-2P  
120021-57-0P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as intermediate for bactericide)
- IT 107-30-2, Methoxymethyl chloride 116-11-0 994-30-9, Triethylsilyl  
chloride 3970-21-6, Methoxyethoxymethyl chloride 25512-65-6,  
Dihydropyran 58479-61-1, tert-Butyldiphenylsilyl chloride  
RL: RCT (Reactant)  
(protection by, of hydroxylysine deriv., in prepn. of bactericide)
- IT 111305-66-9 111305-70-5 111337-87-2 119962-92-4 119962-94-6  
120021-56-9  
RL: RCT (Reactant)  
(reaction of, in prepn. of bactericide)
- IT 867-44-7 34670-47-8, 1-Methylhydrazinoacetic acid 51127-12-9  
119976-93-1  
RL: RCT (Reactant)  
(reaction of, in prepn. of hydroxylysine bactericide)
- IT 75-77-4, Trimethylsilyl chloride, reactions 2986-19-8,  
S-Methylisothiourrea 22509-74-6, N-Carboethoxyphthalimide  
RL: RCT (Reactant)  
(reaction of, with hydroxylysine deriv., in prepn. of bactericide)
- IT 86-81-7, 3,4,5-Trimethoxybenzaldehyde  
RL: RCT (Reactant)  
(reductive alkylation by, of hydroxylysine deriv., in prepn. of  
bactericide)
- IT 100-52-7, Benzaldehyde, reactions  
RL: RCT (Reactant)  
(reductive alkylation by, of hydroxylysine deriv., in prepn. of sodium  
cyanoborohydride)
- IT 75-07-0, Acetaldehyde, reactions  
RL: RCT (Reactant)  
(reductive ethylation by, of amino acid deriv., in presence of sodium  
cyanoborohydride)
- IT 50-00-0, Formaldehyde, reactions  
RL: RCT (Reactant)  
(reductive methylation of amino acid by, in the presence of sodium  
cyanoborohydride)
- IT 110-60-1, 1,4-Butanediamine  
RL: RCT (Reactant)  
(ring-opening by, of .delta.-lactone)
- IT 119960-51-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation)  
(prepn. and deprotection of, in prepn. of bactericide)
- RN 119960-51-9 HCAPLUS
- CN L-threo-Hexonamide, 6-[[3-[(aminocarbonyl)oxy]-2-[[[(1,1-  
dimethylethoxy)carbonyl]amino]-1-oxopropyl]amino]-N-(3-amino-3-  
iminopropyl)-2,3,4,6-tetraeoxy-3-[[[(1,1-dimethylethoxy)carbonyl]amino]-,  
monohydrochloride, (S)- (9CI) (CA INDEX NAME)

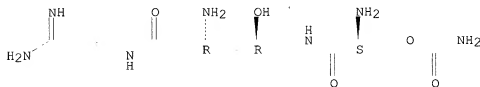
Absolute stereochemistry.



● HCl

IT 119961-60-3P  
 RL: BAC (Biological activity or effector, except adverse); SPN  
 (Synthetic preparation); BIOL (Biological study); PREP  
 (Preparation)  
 (prepn. of, as bactericide)  
 RN 119961-60-3 HCAPLUS  
 CN L-threo-Hexonamide, 3-amino-6-[[2-amino-3-[(aminocarbonyl)oxy]-1-  
 oxopropyl]amino]-N-(3-amino-3-iminopropyl)-2,3,4,6-tetra-deoxy-,  
 trihydrochloride, (S)- (9CI) (CA INDEX NAME)

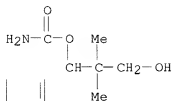
Absolute stereochemistry.



●3 HCl

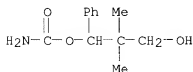
L33 ANSWER 9 OF 13 HCAPLUS COPYRIGHT 2002 ACS  
 AN 1972:419419 HCAPLUS  
 DN 77:19419  
 TI Chloroformate and carbonate derivatives of substituted and unsubstituted  
 1-phenyl-2,2-dialkyl-1,3-dihydroxypropanes  
 IN Kulka, Kurt  
 PA Fritzsche Dodge and Olcott Inc.  
 SO U.S., 10 pp. Division of U.S. 3,415,844 (CA 71;91102q).  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC C07C; A61K  
 NCL 260463000  
 CC 25-21 (Noncondensed Aromatic Compounds)  
 FAN.CNT 1  
 PATENT NO. KIND DATE APPLICATION NO. DATE  
 -----

PI US 3629314 A 19711221 US 1968-761875 19680923  
 GI For diagram(s), see printed CA Issue.  
 AB Monocarbonates (I) (R = H, OMe, Me2CH, Me, Cl; R1 = H or RR1 = OCH2O; R2 = H or CONH2 .noteq. R3 = H or CONH2) were prepd. from the corresponding propanediols by treatment with ClCO2R (R = Et or Me) and Me3N to give the corresponding monoalkyl and cyclic carbonates and then **ammonolysis** of the carbonates. The monocarbonates were potential tranquilizers.  
 ST carbamate tranquilizer; propanediol carbamate tranquilizer  
 IT 24020-78-8P **24020-79-9P** 24020-80-2P 24020-81-3P  
 24020-82-4P 24020-83-5P 24020-84-6P 24020-85-7P 24020-86-8P  
 24020-87-9P 24020-88-0P 24020-89-1P 24020-90-4P 24020-91-5P  
 24026-62-8P 24026-65-1P **24026-66-2P** **24026-67-3P**  
 24026-70-8P 24026-75-3P **24026-76-4P** 24063-46-5P  
 35615-31-7P 36088-40-1P 36088-41-2P 36088-42-3P 36088-43-4P  
 RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (prepn. of)  
 IT 33950-46-8  
 RL: RCT (Reactant)  
 (reaction of with phosgene)  
 IT 79-22-1  
 RL: RCT (Reactant)  
 (reaction of, with (methoxyphenyl)dimethyldihydroxypropane)  
 IT 103-71-9  
 RL: RCT (Reactant)  
 (reaction of, with (methylenedioxy)phenyl-2,2-dimethyldihydroxypropane)  
 IT 24793-94-0 35615-33-9  
 RL: RCT (Reactant)  
 (reaction of, with ethyl chloroformate)  
 IT 35613-25-3  
 RL: RCT (Reactant)  
 (reaction of, with ethyl isocyanate)  
 IT 35615-32-8  
 RL: RCT (Reactant)  
 (reaction of, with ethylchloroformate)  
 IT 24793-83-7  
 RL: RCT (Reactant)  
 (reaction of, with methyl chloroformate)  
 IT 109-90-0  
 RL: RCT (Reactant)  
 (reaction of, with naphthyldimethyldihydroxypropane)  
 IT 75-44-5  
 RL: RCT (Reactant)  
 (reaction of, with phenyldimethyldihydroxypropane)  
 IT 31758-87-9  
 RL: RCT (Reactant)  
 (reaction of, with phosgene)  
 IT **24020-79-9P** **24026-66-2P** **24026-67-3P**  
**24026-76-4P**  
 RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (prepn. of)  
 RN 24020-79-9 HCAPLUS  
 CN 1,3-Propanediol, 1-(4-chlorophenyl)-2,2-dimethyl-, 1-carbamate (9CI) (CA  
 INDEX NAME)

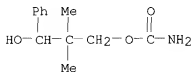


Cl

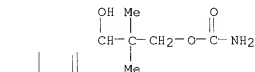
RN 24026-66-2 HCAPLUS  
 CN 1,3-Propanediol, 2,2-dimethyl-1-phenyl-, 1-carbamate (8CI, 9CI) (CA INDEX NAME)



RN 24026-67-3 HCAPLUS  
 CN 1,3-Propanediol, 2,2-dimethyl-1-phenyl-, 3-carbamate (8CI, 9CI) (CA INDEX NAME)



RN 24026-76-4 HCAPLUS  
 CN 1,3-Propanediol, 1-(4-chlorophenyl)-2,2-dimethyl-, 3-carbamate (9CI) (CA INDEX NAME)



Cl

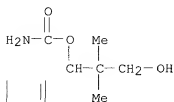
L33 ANSWER 10 OF 13 HCAPLUS COPYRIGHT 2002 ACS  
 AN 1972:405217 HCAPLUS  
 DN 77:5217  
 TI Monocarbamates and n-alkyl or N-phenyl monocarbamates of substituted and unsubstituted 1-phenyl-2,2-dialkyl-1,3-dihydroxypropanes  
 IN Kulka, Kurt  
 PA Fritzsche Dodge and Olcott Inc.  
 SO U.S., 11 pp. Division of U.S. 3,415,844 (CA 71:91102g).  
 CODEN: USXXAM

DT Patent  
 LA English  
 IC C07D  
 NCL 260340500  
 CC 25-21 (Noncondensed Aromatic Compounds)  
 Section cross-reference(s): 28

FAN.CNT 1

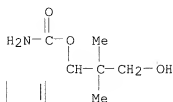
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3637753	A	19720125	US 1968-761797	19680923
GI	For diagram(s), see printed CA Issue.				
AB	Division of U.S. 3,415,844 (CA 71: 91102q). The title compds., useful animal relaxants, were prepd. Thus, 1-(4-methoxyphenyl)-2,2-dimethyl-1,3-dihydroxypropane (I), MeO2CCl, pyridine, and C6H6 was stirred 1 hr and then heated 5 hr at 52-62.degree. to give 15-20% of the <b>cyclic</b> carbonate (II, R = 4-MeO) of I. <b>NH3</b> (g) was passed 17 hr into a soln. of II in aq. <b>NH3</b> -isopropanol to give a mixt. of mono carbamates RC6H4CH(O2CNHR1)CMe2CH2OH (III, R = 4-MeO, R1 = H) and RC6H4CH(OH)CMe2CH2O2CNHR1 (IV, R = 4-MeO, R1 = H). Similarly prepd. were .apprx.10 analogs of II as well as .apprx.10 carbamate mixts. including III (R = H, R1 = Ph) and IV (R = H, R1 = Ph).				
ST	carbamate phenyl hydroxypropane; carbonate phenyl hydroxypropane				
IT	24020-78-8P	<b>24020-79-9P</b>	24020-80-2P	24020-81-3P	
	24020-82-4P	24020-83-5P	24020-84-6P	24020-90-4P	24020-91-5P
	24020-92-6P	24020-93-7P	24026-60-6P	24026-61-7P	24026-62-8P
	<b>24026-63-9P</b>	<b>24026-64-0P</b>	24026-65-1P		
	<b>24026-66-2P</b>	<b>24026-67-3P</b>	24026-68-4P	24026-69-5P	
	24026-70-8P	<b>24026-71-9P</b>	<b>24026-72-0P</b>	24026-73-1P	
	24026-74-2P	24026-75-3P	<b>24026-76-4P</b>	24026-77-5P	
	24026-78-6P	<b>24063-00-1P</b>	<b>24063-01-2P</b>	24793-83-7P	
	24793-94-0P	25321-45-3P	25321-46-4P	25321-47-5P	<b>25321-48-6P</b>
	<b>25321-49-7P</b>	25897-12-5P	36851-20-4P	36851-21-5P	
	36851-22-6P	36851-23-7P	36911-07-6P	36911-08-7P	
	RL: <b>SPN (Synthetic preparation)</b> ; <b>PREP (Preparation)</b> (prepn. of)				
IT	36851-29-3				
	RL: RCT (Reactant) (reaction of, with ammonia and phosgene)				
IT	78-84-2				
	RL: RCT (Reactant) (reaction of, with benzaldehydes)				
IT	31758-87-9	33950-46-8	35613-25-3	35615-33-9	36851-35-1
	RL: RCT (Reactant) (reaction of, with chloroformates)				
IT	122-03-2	123-11-5	1334-78-7		
	RL: RCT (Reactant) (reaction of, with isobutyraldehyde)				
IT	75-44-5	79-22-1	103-71-9	109-90-0	541-41-3 624-83-9
	RL: RCT (Reactant) (reaction of, with phenyldihydroxypropanes)				
IT	<b>7664-41-7</b> , reactions				
	RL: RCT (Reactant) (with carbonate and formate esters)				
IT	<b>24020-79-9P</b>	<b>24026-63-9P</b>	<b>24026-64-0P</b>		
	<b>24026-66-2P</b>	<b>24026-67-3P</b>	<b>24026-71-9P</b>		
	<b>24026-72-0P</b>	<b>24026-76-4P</b>	<b>24063-00-1P</b>		
	<b>24063-01-2P</b>	<b>25321-48-6P</b>	<b>25321-49-7P</b>		
	RL: <b>SPN (Synthetic preparation)</b> ; <b>PREP (Preparation)</b> (prepn. of)				
RN	24026-79-9	HCAPLUS			

CN 1,3-Propanediol, 1-(4-chlorophenyl)-2,2-dimethyl-, 1-carbamate (9CI) (CA INDEX NAME)



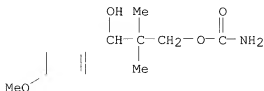
Cl

RN 24026-63-9 HCAPLUS  
CN 1,3-Propanediol, 1-(4-methoxyphenyl)-2,2-dimethyl-, 1-carbamate (9CI) (CA INDEX NAME)



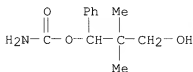
MeO

RN 24026-64-0 HCAPLUS  
CN 1,3-Propanediol, 1-(4-methoxyphenyl)-2,2-dimethyl-, 3-carbamate (9CI) (CA INDEX NAME)



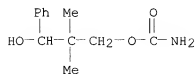
MeO

RN 24026-66-2 HCAPLUS  
CN 1,3-Propanediol, 2,2-dimethyl-1-phenyl-, 1-carbamate (8CI, 9CI) (CA INDEX NAME)

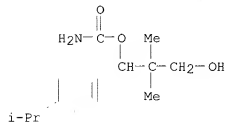


RN 24026-67-3 HCAPLUS  
CN 1,3-Propanediol, 2,2-dimethyl-1-phenyl-, 3-carbamate (8CI, 9CI) (CA INDEX NAME)

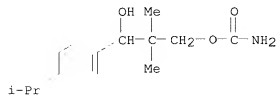




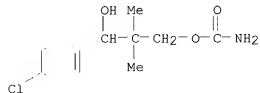
RN 24026-71-9 HCAPLUS  
 CN 1,3-Propanediol, 2,2-dimethyl-1-[4-(1-methylethyl)phenyl]-, 1-carbamate (9CI) (CA INDEX NAME)



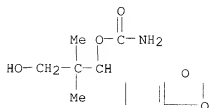
RN 24026-72-0 HCAPLUS  
 CN 1,3-Propanediol, 2,2-dimethyl-1-[4-(1-methylethyl)phenyl]-, 3-carbamate (9CI) (CA INDEX NAME)



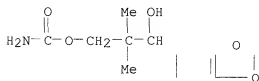
RN 24026-76-4 HCAPLUS  
 CN 1,3-Propanediol, 1-(4-chlorophenyl)-2,2-dimethyl-, 3-carbamate (9CI) (CA INDEX NAME)



RN 24063-00-1 HCAPLUS  
 CN 1,3-Propanediol, 1-(1,3-benzodioxol-5-yl)-2,2-dimethyl-, 1-carbamate (9CI) (CA INDEX NAME)



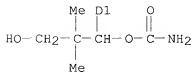
RN 24063-01-2 HCAPLUS  
 CN 1,3-Propanediol, 1-(1,3-benzodioxol-5-yl)-2,2-dimethyl-, 3-carbamate (9CI)  
 (CA INDEX NAME)



RN 25321-48-6 HCAPLUS  
 CN 1,3-Propanediol, 2,2-dimethyl-1-(methylphenyl)-, 1-carbamate (9CI) (CA  
 INDEX NAME)

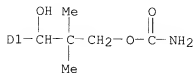


D1-Me



RN 25321-49-7 HCAPLUS  
 CN 1,3-Propanediol, 2,2-dimethyl-1-(methylphenyl)-, 3-carbamate (9CI) (CA  
 INDEX NAME)

D1-Me



IT 7664-41-7, reactions  
 RL: RCT (Reactant)  
 (with carbonate and formate esters)  
 RN 7664-41-7 HCAPLUS  
 CN Ammonia (8CI, 9CI) (CA INDEX NAME)

NH3

L33 ANSWER 11 OF 13 HCAPLUS COPYRIGHT 2002 ACS

AN 1970:21476 HCAPLUS

DN 72:21476

TI Hypnotic and tranquilizing 1-aryl-2,2-dialkyl-1,3-dihydroxypropane derivatives

IN Kulka, Kurt

PA Fritzsche Brothers, Inc.

SO S. African, 46 pp.

CODEN: SFXXAB

DT Patent

LA English

CC 25 (Noncondensed Aromatic Compounds)

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	ZA 6704670		19690203	ZA	19670803

GI For diagram(s), see printed CA Issue.

AB p-R1C6H4CH(OR2)CMeCH2OR3 (I) and II (R = Me or Pr, R1 = H, Me, MeO, iso-Pr, or Cl, R2 and R3 = H, CO2Me, CO2Et, cONH2, CONHMe, CONHEt, or CONHPh), having sedative, hypnotic, and tranquilizing activities are prepd. from I (R2 = R3 = H). For example, 140 g 85% methanolic KOH was treated with a mixt. of 272 g p-MeOC6H4CHO and 360 g iso-PrCHO over 1.5 hr at 44-9.degree., stirred at 42.degree. for 3 hr, cooled to 30.degree., acidified (AcOH), concd. to remove 250 ml MeOH, and dild. with water to sep. 65.5% I (R = Me, R1 = MeO, R2 = R3 = H) (III), b6 178-93.degree., m. 71.5-2.degree.. A mixt. of 50 g III, 70 ml benzene, and 26 g pyridine was treated with 37 g ClCO2Me in 30 ml benzene at 18-25.degree. over 45 min, stirred at room temp. and 52-62.degree. for 1 and 5 hr, resp. to give a mixt. of monomethyl and cyclic carbonates of III. II (R = Me, R1 = MeO, 15-20%), m. 138-9.degree., was crystd. from iso-PrOH. Introduction of NH3 into a mixt. of 55 g III, 80 ml iso-PrOH and

30 ml 28% aq.  $\text{NH}_3$  at room temp. for 17 hr gave 50 g monocarbamate mixt. of III. A soln. of 218 g COCl<sub>2</sub> in 2 l. toluene was treated with 180 g I (R = Me, R<sub>1</sub> = R<sub>2</sub> = R<sub>3</sub> = H) (IV) in 100 g pyridine and 500 ml CHCl<sub>3</sub> at -1-4.degree. over 12.5 hr to give, after 17 hr, 90% II (R = Me, R<sub>1</sub> = H) (V), m. 112-14.degree.. Treatment of V with  $\text{NH}_3$  gave 54.2% monocarbamate mixt. of IV. A soln. of 214 g I (R = Me, R<sub>1</sub> = Cl, R<sub>2</sub> = R<sub>3</sub> = H) (VI) in 400 ml tetrahydrofuran contg. 125 g PhNMe<sub>2</sub> was added to 104 g COCl<sub>2</sub> in 200 ml toluene at -5.degree., cooled to -7.degree., treated with 2 moles 28-30% aq.  $\text{NH}_3$  to give, after removal of PhNMe<sub>2</sub> by steam distn., 50-58% I (R = Me, R<sub>1</sub> = Cl, R<sub>2</sub> = H, R<sub>3</sub> = CONH<sub>2</sub>), m. 134.degree.. Treatment of 0.5 mole VI and 0.54 mole Et<sub>3</sub>N in 150 ml benzene with 0.55 mole ClCO<sub>2</sub>Et gave 137.5 g monoethyl carbonate mixt. of VI, which was heated at 120-70.degree./6-7 mm for 20 hr to give 82.1 g II (R = Me, R<sub>1</sub> = Cl,) (VII), m. 120-3.degree.. Treatment of 240 g VII in 360 ml iso-PrOH contg. 100 ml 28-30% aq.  $\text{NH}_3$  with  $\text{NH}_3$  for 18 hr at 35-40.degree. gave 45% I (R = Me, R<sub>1</sub> = Cl, R<sub>2</sub> = CONH<sub>2</sub>, R<sub>3</sub> = H), m. 171.degree.. A soln. of 180 g IV in 200 ml tetrahydrofuran was treated with a soln. of 62.7 g MeNCO in 100 ml tetrahydrofuran followed by 3 drops pyridine to give, after 24 hr 70% monomethylcarbamate mixt. of IV. Acetylation of 53.6 g VI with 16.5 g AcOH in 150 ml toluene contg. 0.25 g p-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H gave 80% I (R = Me, R<sub>1</sub> = Cl, R<sub>2</sub> = H, R<sub>3</sub> = Ac), m. 78.5-80.degree.. Treatment of I (R = Me, R<sub>1</sub> = R<sub>2</sub> = H, R<sub>3</sub> = Ac) (VIII) and Et<sub>3</sub>N in toluene with COCl<sub>2</sub> followed by  $\text{NH}_3$  and subsequent hydrolysis gave I (R = Me, R<sub>1</sub> = R<sub>3</sub> = H, R<sub>2</sub> = CONH<sub>2</sub>). Treatment of VIII and Et<sub>3</sub>N in toluene with ClCO<sub>2</sub>Et followed by  $\text{NH}_3$  and subsequent hydrolysis gave I (R = Me, R<sub>1</sub> = R<sub>3</sub> = H, R<sub>2</sub> = CONH<sub>2</sub>). Other compds. such as derivs. of 1-(3,4-methylenedioxyphenyl)- and 1-(1-naphthyl)-2,2-dimethyl-1,3-dihydroxypropanes are also similarly prepd.

ST benzenes dihydroxypropyl substituted; hypnotic dihydroxypropylbenzenes; dihydroxypropylbenzenes hypnotic; tranquilizers dihydroxypropylbenzenes

IT 24020-78-8P 24020-79-9P 24020-80-2P 24020-81-3P  
24020-82-4P 24020-83-5P 24020-84-6P 24020-85-7P 24020-86-8P  
24020-87-9P 24020-88-0P 24020-89-1P 24020-90-4P 24020-91-5P  
24020-92-6P 24020-93-7P 24026-60-6P 24026-61-7P 24026-62-8P  
24026-63-9P 24026-64-0P 24026-65-1P  
24026-66-2P 24026-67-3P 24026-68-4P 24026-69-5P  
24026-70-8P 24026-71-9P 24026-72-0P 24026-73-1P  
24026-74-2P 24026-75-3P 24026-76-4P 24026-77-5P  
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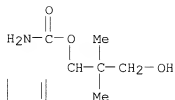
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

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24026-72-0P 24026-76-4P 24063-00-1P 24063  
-01-2P 25321-48-6P 25321-49-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 24020-79-9 HCAPLUS

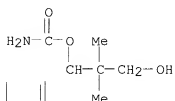
CN 1,3-Propanediol, 1-(4-chlorophenyl)-2,2-dimethyl-, 1-carbamate (9CI) (CA INDEX NAME)



Cl

RN 24026-63-9 HCAPLUS

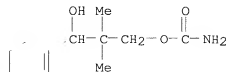
CN 1,3-Propanediol, 1-(4-methoxyphenyl)-2,2-dimethyl-, 1-carbamate (9CI) (CA INDEX NAME)



MeO

RN 24026-64-0 HCAPLUS

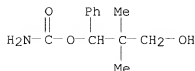
CN 1,3-Propanediol, 1-(4-methoxyphenyl)-2,2-dimethyl-, 3-carbamate (9CI) (CA INDEX NAME)



MeO

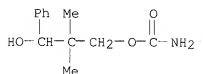
RN 24026-66-2 HCAPLUS

CN 1,3-Propanediol, 2,2-dimethyl-1-phenyl-, 1-carbamate (8CI, 9CI) (CA INDEX NAME)



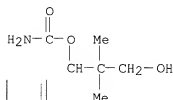
RN 24026-67-3 HCAPLUS

CN 1,3-Propanediol, 2,2-dimethyl-1-phenyl-, 3-carbamate (8CI, 9CI) (CA INDEX NAME)



RN 24026-71-9 HCAPLUS

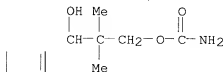
CN 1,3-Propanediol, 2,2-dimethyl-1-[4-(1-methylethyl)phenyl]-, 1-carbamate (9CI) (CA INDEX NAME)



i-Pr

RN 24026-72-0 HCAPLUS

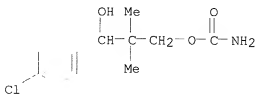
CN 1,3-Propanediol, 2,2-dimethyl-1-[4-(1-methylethyl)phenyl]-, 3-carbamate (9CI) (CA INDEX NAME)



i-Pr

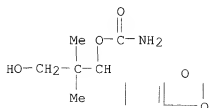
RN 24026-76-4 HCAPLUS

CN 1,3-Propanediol, 1-(4-chlorophenyl)-2,2-dimethyl-, 3-carbamate (9CI) (CA INDEX NAME)



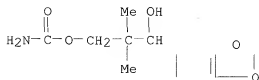
RN 24063-00-1 HCAPLUS

CN 1,3-Propanediol, 1-(1,3-benzodioxol-5-yl)-2,2-dimethyl-, 1-carbamate (9CI) (CA INDEX NAME)



RN 24063-01-2 HCAPLUS

CN 1,3-Propanediol, 1-(1,3-benzodioxol-5-yl)-2,2-dimethyl-, 3-carbamate (9CI)  
(CA INDEX NAME)

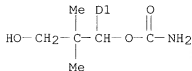


RN 25321-48-6 HCAPLUS

CN 1,3-Propanediol, 2,2-dimethyl-1-(methylphenyl)-, 1-carbamate (9CI) (CA  
INDEX NAME)



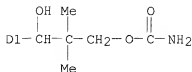
D1-Me



RN 25321-49-7 HCAPLUS

CN 1,3-Propanediol, 2,2-dimethyl-1-(methylphenyl)-, 3-carbamate (9CI) (CA  
INDEX NAME)

D1-Me



L33 ANSWER 12 OF 13 HCAPLUS COPYRIGHT 2002 ACS

AN 1969:491101 HCAPLUS

DN 71:91101

TI Derivatives of glycol carbonates and carbamates

PA Fritzsche Brothers, Inc.

SO Fr., 16 pp.

CODEN: FRXXAK

DT Patent

LA French

IC C07C; A61K

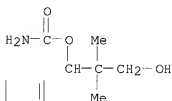
CC 25 (Noncondensed Aromatic Compounds)

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 1534503		19680726	FR	19670821
AB	1-Phenyl-2,2-dialkyl-1,3-dihydroxypropanes, and their derivs, substituted in the C6H6 ring, were converted into carbonates, carbamates and N-substituted carbamates. Thus, 4-ClC6H4CH(OH)CMe2CH2OH, treated successively with COCl2 and NH3 gave 4-ClC6H4CH(OH)CMe2CH2OCONH2.				
ST	carbonates glycol; glycol carbonates; carbamates glycol				
IT	24020-78-8P	24020-79-9P	24020-80-2P	24020-81-3P	
	24020-82-4P	24020-83-5P	24020-84-6P	24020-85-7P	24020-86-8P
	24020-87-9P	24020-88-0P	24020-89-1P	24020-90-4P	24020-91-5P
	24020-92-6P	24020-93-7P	24026-60-6P	24026-61-7P	24026-62-8P
	24026-63-9P	24026-64-0P	24026-65-1P		
	24026-66-2P	24026-67-3P	24026-68-4P	24026-69-5P	
	24026-70-8P	24026-71-9P	24026-72-0P	24026-73-1P	
	24026-74-2P	24026-75-3P	24026-76-4P	24026-77-5P	
	24026-78-6P	24063-00-1P	24063-01-2P	24063-46-5P	
	25321-45-3P	25321-46-4P	25321-47-5P	25321-48-6P	
	25321-49-7P				
RL:	SPN (Synthetic preparation); PREP (Preparation) (prepn. of)				
IT	24020-79-9P	24026-63-9P	24026-64-0P		
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	24026-72-0P	24026-76-4P	24063-00-1P		
	24063-01-2P	25321-48-6P	25321-49-7P		
RL:	SPN (Synthetic preparation); PREP (Preparation) (prepn. of)				
RN	24020-79-9	HCAPLUS			



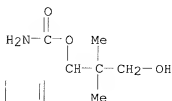
CN 1,3-Propanediol, 1-(4-chlorophenyl)-2,2-dimethyl-, 1-carbamate (9CI) (CA INDEX NAME)



Cl

RN 24026-63-9 HCAPLUS

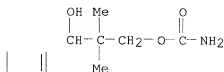
CN 1,3-Propanediol, 1-(4-methoxyphenyl)-2,2-dimethyl-, 1-carbamate (9CI) (CA INDEX NAME)



MeO

RN 24026-64-0 HCAPLUS

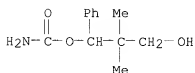
CN 1,3-Propanediol, 1-(4-methoxyphenyl)-2,2-dimethyl-, 3-carbamate (9CI) (CA INDEX NAME)



MeO

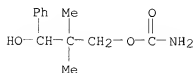
RN 24026-66-2 HCAPLUS

CN 1,3-Propanediol, 2,2-dimethyl-1-phenyl-, 1-carbamate (8CI, 9CI) (CA INDEX NAME)



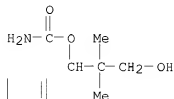
RN 24026-67-3 HCAPLUS

CN 1,3-Propanediol, 2,2-dimethyl-1-phenyl-, 3-carbamate (8CI, 9CI) (CA INDEX NAME)



RN 24026-71-9 HCAPLUS

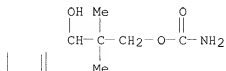
CN 1,3-Propanediol, 2,2-dimethyl-1-[4-(1-methylethyl)phenyl]-, 1-carbamate (9CI) (CA INDEX NAME)



i-Pr

RN 24026-72-0 HCAPLUS

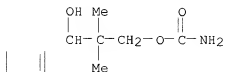
CN 1,3-Propanediol, 2,2-dimethyl-1-[4-(1-methylethyl)phenyl]-, 3-carbamate (9CI) (CA INDEX NAME)



i-Pr

RN 24026-76-4 HCAPLUS

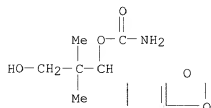
CN 1,3-Propanediol, 1-(4-chlorophenyl)-2,2-dimethyl-, 3-carbamate (9CI) (CA INDEX NAME)



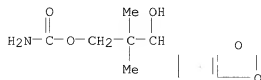
Cl

RN 24063-00-1 HCAPLUS

CN 1,3-Propanediol, 1-(1,3-benzodioxol-5-yl)-2,2-dimethyl-, 1-carbamate (9CI) (CA INDEX NAME)



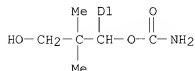
RN 24063-01-2 HCAPLUS

CN 1,3-Propanediol, 1-(1,3-benzodioxol-5-yl)-2,2-dimethyl-, 3-carbamate (9CI)  
(CA INDEX NAME)

RN 25321-48-6 HCAPLUS

CN 1,3-Propanediol, 2,2-dimethyl-1-(methylphenyl)-, 1-carbamate (9CI) (CA  
INDEX NAME)

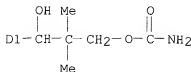
D1-Me



RN 25321-49-7 HCAPLUS

CN 1,3-Propanediol, 2,2-dimethyl-1-(methylphenyl)-, 3-carbamate (9CI) (CA  
INDEX NAME)

Dl-Me



L33 ANSWER 13 OF 13 HCAPLUS COPYRIGHT 2002 ACS

AN 1969:412494 HCAPLUS

DN 71:12494

TI Carbamate derivatives related to meprobamate

AU Ludwig, Bernard J.; Powell, Leo S.; Berger, Frank Milan

CS Wallace Lab., Carter-Wallace, Inc., Cranbury, N. J., USA

SO J. Med. Chem. (1969), 12(3), 462-72

CODEN: JMCMAR

DT Journal

LA English

CC 23 (Aliphatic Compounds)

AB A series of 2-substituted 1,3-propanediol dicarbamates, related chem. to meprobamate, was prepd. for central nervous system pharmacol. investigation. The N-unsubstituted propanediol dicarbamates were obtained by an ester-exchange reaction between the corresponding diol and urethane, by phosgenation of the diol followed by **ammoniation** of the bis(chlorocarbonate) deriv., by the reaction of the diol with cyanic acid, and by **ammoniation** of the bis(phenylcarbonate) deriv. of the appropriate diol. The sym. N,N'-substituted propanediol dicarbamates were synthesized by direct carbamoylation of the propanediols, and the unsym. substituted derivs. by stepwise carbamoylation via the m-**dioxanone** and hydroxypropyl carbamate intermediates using similar carbamoylation reactions. In addn. to the prepn. and phys. properties of these compds., the muscle paralyzing activity, anticonvulsant activity, and toxicity of these carbamates and many of the intermediates employed in their synthesis are presented. Structure-activity relations among these compds. are discussed.

ST propanediols carbamoylation; carbamoylation propanediols

IT Antispasmodics

IT Muscles, responses to chemicals  
(to propanediol carbamate derivs.)

IT 1,3-Propanediol, 2,2-diphenyl-, dicarbamate

1,3-Propanediol, 2-methyl-2-propyl-, bis(1-aziridinecarboxylate)

1,3-Propanediol, 2-sec-butyl-2-methyl-, carbamate carbazate (ester)

1-Aziridinecarboxylic acid, 2-methyl-2-propyltrimethylene ester

Carbazic acid, 2-(hydroxymethyl)-2,3-dimethylpentyl ester carbamate (ester)

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

IT 57-53-4P 64-55-1P 78-44-4P 1146-18-5P 1672-81-7P 1672-86-2P

1729-14-2P 2037-62-9P 2109-29-7P 2109-30-0P 2109-88-8P

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RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

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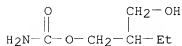
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RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

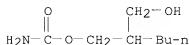
IT 25451-51-8P 25451-52-9P 25451-53-0P  
 25451-54-1P 25451-55-2P 25451-56-3P  
 25451-57-4P 25451-58-5P 25451-59-6P  
 25451-60-9P 25451-61-0P 25451-62-1P  
 25451-63-2P 25451-64-3P 25480-69-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

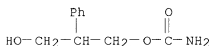
RN 25451-51-8 HCAPLUS  
 CN 1,3-Propanediol, 2-ethyl-, monocarbamate (8CI) (CA INDEX NAME)



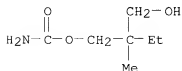
RN 25451-52-9 HCAPLUS  
 CN 1,3-Propanediol, 2-butyl-, monocarbamate (8CI) (CA INDEX NAME)



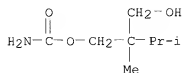
RN 25451-53-0 HCAPLUS  
 CN 1,3-Propanediol, 2-phenyl-, monocarbamate (8CI, 9CI) (CA INDEX NAME)



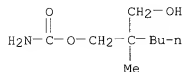
RN 25451-54-1 HCAPLUS  
 CN 1,3-Propanediol, 2-ethyl-2-methyl-, monocarbamate (8CI) (CA INDEX NAME)



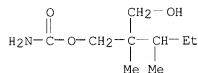
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 CN 1,3-Propanediol, 2-isopropyl-2-methyl-, monocarbamate (8CI) (CA INDEX NAME)



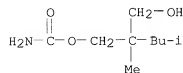
RN 25451-56-3 HCAPLUS  
CN 1,3-Propanediol, 2-butyl-2-methyl-, monocarbamate (8CI) (CA INDEX NAME)



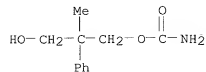
RN 25451-57-4 HCAPLUS  
CN 1,3-Propanediol, 2-sec-butyl-2-methyl-, monocarbamate (8CI) (CA INDEX NAME)



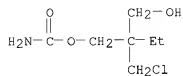
RN 25451-58-5 HCAPLUS  
CN 1,3-Propanediol, 2-isobutyl-2-methyl-, monocarbamate (8CI) (CA INDEX NAME)



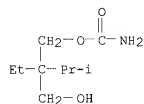
RN 25451-59-6 HCAPLUS  
CN 1,3-Propanediol, 2-methyl-2-phenyl-, monocarbamate (8CI) (CA INDEX NAME)-----



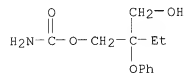
RN 25451-60-9 HCAPLUS  
CN 1,3-Propanediol, 2-(chloromethyl)-2-ethyl-, monocarbamate (8CI) (CA INDEX NAME)



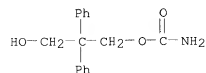
RN 25451-61-0 HCAPLUS  
CN 1,3-Propanediol, 2-ethyl-2-isopropyl-, monocarbamate (8CI) (CA INDEX NAME)



RN 25451-62-1 HCAPLUS  
CN 1,3-Propanediol, 2-ethyl-2-phenoxy-, monocarbamate (8CI) (CA INDEX NAME)

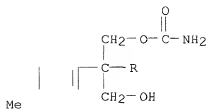


RN 25451-63-2 HCAPLUS  
CN 1,3-Propanediol, 2,2-diphenyl-, monocarbamate (8CI) (CA INDEX NAME)



RN 25451-64-3 HCAPLUS  
CN 1,3-Propanediol, 2,2-di-p-tolyl-, monocarbamate (8CI) (CA INDEX NAME)





RN 25480-69-7 HCAPLUS  
 CN 1,3-Propanediol, 2-ethyl-2-propyl-, monocarbamate (8CI) (CA INDEX NAME)

